# Soft X-ray Absorption and Emission Studies of Titanium Dioxide Powders

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Abstract No. mcgu3499
Beamline(s): **X1B**

**Introduction**: This is a preliminary step in the investigation of whether size effects can be observed in the soft x-ray emission and soft x-ray absorption spectra of $TiO_2$ samples. Furthermore, there is currently great research interest in titanium dioxide for its use as a nanocrystalline mesoporous membrane which may be used as a matrix for building more efficient solar cells through dye sensitization techniques.

**Methods and Materials**: Soft X-ray emission (SXE) spectroscopy is a sensitive tool which probes the LPDOS of the valence band. The high-intensity soft x-ray undulator beamline X1B combined with a specially designed soft x-ray emission spectrometer is ideally suited for use with this photon in-photon out spectroscopy.

Various size distributions of $TiO_2$ powders in the rutile crystal phase have been used in these preliminary experiments. The results reported here have been obtained from powders with median particle sizes of 1.0μm and 0.17μm. Results obtained from true nanocrystals (sizes of ~20nm) of $TiO_2$ suspended in liquid have not been included in this preliminary report.

**Results**: The soft x-ray emission spectra reported here are compared to previously reported spectra obtained by Finkelstein *et al.* Shown in **Figure 1** is a typical SXA and SXE spectrum obtained from $TiO_2$ of 1.0μm size. A comparison of the SXA spectra for the 0.17μm and 1.0μm $TiO_2$ powders is shown for the O 1s edge in **Figure 2** and the Ti 2p edge in **Figure 3**. A plot of the excitation energy dependence of the Ti L2,3 emission is shown in **Figure 4** and follows closely to that observed for a macroscopic single crystal by Finkelstein *et al.*

**Conclusions**: For the range of particle sizes included in this report there are no significant deviations between the previously reported O *1s* SXE of $TiO_2$ and the current measurements. Nor are there significant differences between the Ti 2p SXE of TiO2 previously reported and our current measurements. We are currently evaluating the minor differences observed in the SXA spectra between the two powder sizes. We intend to extend our measurements in collaboration with others to obtain results from suspended nanocrystals of $TiO_2$ in the near future.

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**References**: L.D. Finkelstein *et al.*, "Electronic structure: Wide-band, narrow-band, and strongly correlated systems - Band approach to the excitation-energy dependence of x-ray fluorescence of $TiO_2$", Physical Review B, 60, no. 4, 2212, 1999.

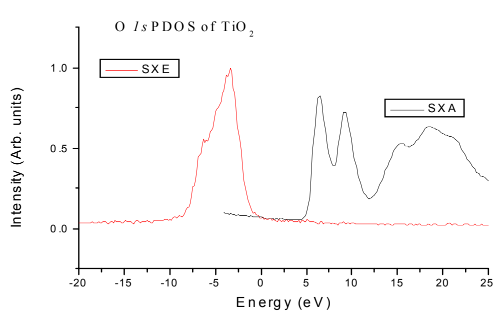


**Figure 1**. The O *K* SXE spectrum of $TiO_2$ of 1.0μm median size combined with the O *K* SXA spectrum. The energy is with respect to valence band maximum (VBM).

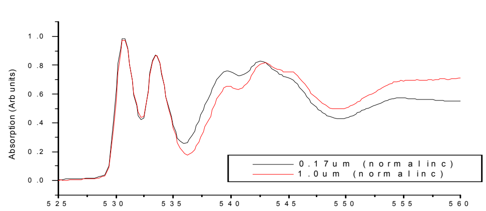


**Figure 2**. Comparison of the O *K* SXA spectrum of $TiO_2$ of 0.17μm and 1.0μm median sizes.

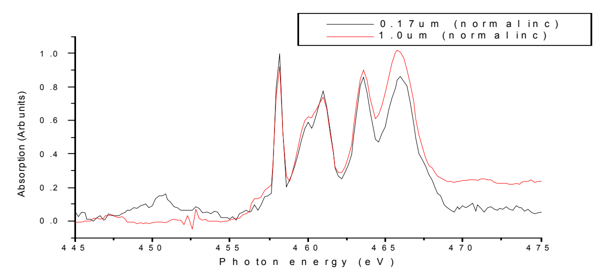


**Figure 3**. Comparison of Ti $L_{2,3}$ SXA spectra from the differently sized $TiO_2$ powders.

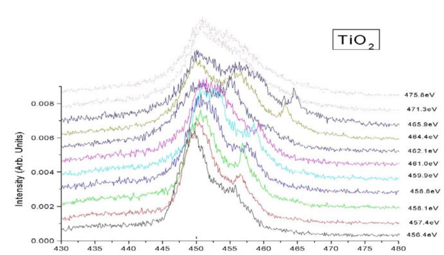


**Figure 4**. Excitation energy dependence of the Ti L2,3 SXE of $TiO_2$ observed from the 0.17μm sized powder.